

3-Amino-1-methyl-5-methylthio-1,2,4-triazole

Inchi:	InChI=1S/C4H8N4S/c1-8-4(9-2)6-3(5)7-8/h1-2H3,(H2,5,7)
InchiKey:	GHBGCSIFUKEXTC-UHFFFAOYSA-N
Formula:	C5H9N3S
SMILES:	CSc1nc(=N)[nH]n1C
Mol. weight [g/mol]:	143.21
CAS:	84827-78-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.48		Crippen Method
logp	-0.532		Crippen Method
mcvol	104.030	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C84827781&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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